

# 15-Digit Accuracy Calculations of Chandrasekhar's $H$ -function for Isotropic Scattering by Means of the Double Exponential Formula

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**Abstract** This work shows that it is possible to calculate numerical values of the Chandrasekhar  $H$ -function for isotropic scattering at least with 15-digit accuracy by making use of the double exponential formula (DE-formula) of Takahashi and Mori (Publ. RIMS, Kyoto Univ. **9**, 721, 1974) instead of the Gauss-Legendre quadrature employed in the numerical scheme of Kawabata and Limaye (Astrophys. Space Sci. **332**, 365, 2011) and simultaneously taking a precautionary measure to minimize the effects due to loss of significant digits particularly in the cases of near-conservative scattering and/or errors involved in returned values of library functions supplied by compilers in use. The results of our calculations are presented for 18 selected values of single scattering albedo  $\varpi_0$  and 22 values of an angular variable  $\mu$ , the cosine of zenith angle  $\theta$  specifying the direction of radiation incident on or emergent from semi-infinite media.

**Keywords** radiative transfer;  $H$ -function; isotropic scattering; double exponential formula

## 1 Introduction

We can express the emergent intensities of radiation reflected by semi-infinite, vertically homogeneous media in terms of Chandrasekhar's  $H$ -functions  $H(\varpi_0, \mu)$ , the solution of the following integral equation:

$$H(\varpi_0, \mu) = 1 + \mu H(\varpi_0, \mu) \int_0^1 \frac{\Psi(\varpi_0, \eta)}{\mu + \eta} H(\varpi_0, \eta) d\eta, \quad (1)$$

where  $\varpi_0$  is the single scattering albedo,  $\mu$  is the cosine of the zenith angle  $\theta$  specifying the direction of incident or emergent direction of radiation, and  $\Psi(\varpi_0, \eta)$  is the characteristic function representing the type of scattering the radiation undergoes (Chandrasekhar 1960). Lately, Kawabata (2015) developed an efficient iterative scheme to obtain numerical values of the  $H(\varpi_0, \mu)$  with 11-digit accuracy by making use of the approximate interpolation formula obtained by Kawabata and Limaye (2011) (see also Kawabata and Limaye 2013, for erratum) for the  $H(\varpi_0, \mu)$  for isotropic scattering, which corresponds to  $\Psi(\varpi_0, \eta) = \frac{1}{2}\varpi_0$ .

Accurate numerical evaluation of the  $H$ -function is important not only for radiative transfer-related problems but also for other disciplinary areas such as the condensed matter physics and the theory of neutron transport as has been pointed out by, e.g., Jablonski (2012). An outstanding work from this standpoint was made by Viik (1986), who succeeded in calculating numerical values of the  $H$ ,  $X$ , and  $Y$ -functions of Chandrasekhar<sup>1</sup> with 14-digit accuracy approximating Sobolev's resolvent function employing exponent series. Equally interesting work was done by Mohankumar and Natarajan (2007), who evaluated the  $H$ -function for isotropic scattering via  $X$ -function of neutron transport for single speed and isotropic case together with the application of the double exponential formula (DE-formula) proposed by Takahashi and Mori (1974).

However, in the case of the  $H$ -function for isotropic scattering, various forms of integral representations such as the one employed by Kawabata and Limaye

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<sup>1</sup>They are often referred to as *Ambarzumian-Chandrasekhar's functions* in Russian literature (see, e.g., Sobolev 1975; Ambarzumian 1942, 1944). However, we shall adhere to the name *Chandrasekhar's functions* just for brevity.

(2011) are known. It would therefore be interesting to investigate if it is possible to calculate the values of the isotropic scattering  $H$ -function using an integral representation with accuracy comparable to that of Viik (1986).

## 2 Formalism

Since our main interest is in applications to radiative transfer problems, we may assume that the parameter  $\varpi_0$  lies in the range  $[0, 1]$ . As in Kawabata and Limaye (2011), let us express the  $H$ -function for isotropic scattering in a closed form:

$$H(\varpi_0, \mu) = \exp \left[ -(\mu/\pi) \int_0^{\pi/2} f_1(\varpi_0, x) f_2(\mu, x) dx \right], \quad (2)$$

where we have defined the functions  $f_1$  and  $f_2$  as

$$f_1(\varpi_0, x) = \ln(1 - \varpi_0 x / \tan x), \quad (3a)$$

$$f_2(\mu, x) = (1 + \tan^2 x) / [1 + (\mu \tan x)^2]. \quad (3b)$$

Evidently,  $H(0, \mu) = 1$  holds irrespective of the values of  $\mu$  due to the fact that  $f_1(0, x) = 0$ .

It should be noted that Kawabata and Limaye (2011) applied the Gauss-Legendre quadrature to perform the integration over the interval  $[0, \pi/2]$  in Eq.(2) for non-conservative cases, viz.,  $\varpi_0 < 1$ . In the conservative case, on the other hand, they partitioned the domain into  $[0, \varepsilon]$  and  $[\varepsilon, \pi/2]$ , and an analytical integration was carried out for the first interval assuming  $\varepsilon \ll 1$ , thereby avoiding the numerical difficulty that would arise from a logarithmic divergence of the integrand at  $x = 0$ , while the Gauss-Legendre quadrature was applied to the second interval.

The most straightforward way to fulfill our objective would therefore be to replace the Gauss-Legendre quadrature with something superior. This premise and the work of Mohankumar and Natarajan (2007) naturally led us to trying the *double exponential formula* (DE-formula) of Takahashi and Mori (1974) for numerical integrations. The optimality of the DE-formula has been mathematically proven by Sugihara (1997), indicating that it is capable of giving the most accurate result by the minimum number of function evaluations (Mori and Sugihara 2001). The method is known to be efficient even for integrals with end-point singularities. Furthermore, it can easily be incorporated with integrations equipped with automatic step-size adjustment. What is more, halving the step-size

approximately doubles the number of significant figures (Takahashi and Mori 1974). Obviously, therefore, the DE-formula is a highly promising alternative to the Gauss-Legendre quadrature employed by Kawabata and Limaye (2011).

In writing our automatic integrator in FORTRAN code applying the DE-formula to calculations of the  $H$ -function, a recourse has been made to the subroutine *DEAUTO*, a RATFOR code, published by Watanabe (1990), which ingeniously circumvents the overflow problem often encountered when computing the weights of the DE-formula (see also Mori 1990). We shall perform all our calculations in double-precision arithmetic with the Compaq Visual Fortran compiler Ver. 6.6 for 32-bit computers.

In actual numerical calculations, we closely follow the procedure of Kawabata and Limaye (2011): for the conservative scattering case ( $\varpi_0 = 1$ ), the integral involved in Eq.(2) is evaluated in two parts as has been mentioned above:

$$H^{\text{DE}}(\varpi_0, \mu) = \exp \left[ -(\mu/\pi) \int_0^{\pi/2} f_1(\varpi_0, x) f_2(\mu, x) dx \right] \\ = \exp [-(\mu/\pi)(I_1 + I_2)], \quad (4)$$

where we have

$$I_1 = \int_0^\varepsilon f_1(\varpi_0, x) f_2(\mu, x) dx \\ \simeq \left\{ (2 \ln \varepsilon - 2 - \ln 3) + \frac{1}{45} [30(1 - \mu^2) \ln \varepsilon \right. \\ + 5\mu^2(2 + 3 \ln 3) - 3(3 + 5 \ln 3)] \varepsilon^2 \\ - \left[ \frac{617}{15750} + \frac{2 \ln 3}{15} - \frac{1}{75} \mu^2(9 + 25 \ln 3) \right. \\ + \frac{1}{25} \mu^4(2 + 5 \ln 3) - \frac{2}{15} (2 - 5\mu^2 + 3\mu^4) \times \\ \left. \left. \times \ln \varepsilon \right] \varepsilon^4 \right\} \varepsilon \quad (5)$$

according to Eq.(A.1) of Kawabata and Limaye (2011), and

$$I_2 = \int_\varepsilon^{\pi/2} f_1(\varpi_0, x) f_2(\mu, x) dx \quad (6)$$

which we shall calculate using an automatic integrator code based on the DE-formula, and hence the suffix DE attached to  $H(\varpi_0, \mu)$  appearing on the left-hand side of Eq.(4). The use of Eq.(5) enables us to avoid the numerical difficulty arising from the logarithmic divergence of  $f_1(1, x)$  as we approach  $x = 0$ .

In the non-conservative cases ( $\varpi_0 < 0$ ), on the other hand, no such singularity problem occurs in the integrand of Eq.(4), so that the DE-formula is applied

to the entire domain  $[0, \pi/2]$  with  $\varepsilon$  being set to 0 in Eq.(6).

Furthermore, to minimize the effect of an error originating from  $f_1(\varpi_0, \mu)$  for small values of  $x$  and that due to loss of significant figures caused when the value of  $\varpi_0$  is close to but not equal to unity, we shall use the Maclaurin series expansion truncated at the  $x^{12}$  order term:

$$1 - \varpi_0 x / \tan x \simeq \delta + \frac{\varpi_0 x^2}{3} \left[ 1 + \frac{x^2}{15} \left[ 1 + \frac{x^2}{21} \left[ 2 + x^2 \left[ \frac{1}{5} + \frac{2x^2}{99} \left[ 1 + \frac{691x^2}{6825} \right] \right] \right] \right] \right], \quad (x \leq x_t < 1), \quad (7)$$

where  $x_t$  is a certain demarcation point and  $\varpi_0 = 1 - \delta$  with  $\delta$  being externally specified. Even for  $x > x_t$ , the use of the following form has been found effective for preventing loss of significant figures:

$$1 - \varpi_0 x / \tan x = 1 - u + u\delta, \quad (8)$$

where we have put  $u = x / \tan x$ .

An adequate set of numerical values for the parameters  $\varepsilon$  and  $x_t$  will be determined applying a modified Powell's method for function minimization (Press et al. 1992) as we shall discuss later. One great advantage of this method is that it does not require gradient of the target function to be minimized.

To check whether or not our values of  $H$ -function have an accuracy of at least 15 decimal figures, we employ an alternative form of the definition equation Eq.(1) (see Eq.(13) on p.107 of Chandrasekhar 1960), and perform a single iteration:

$$H^{\text{It}}(\varpi_0, \mu) = \left[ \sqrt{\delta} + \frac{\varpi_0}{2} \int_0^1 \frac{x H^{\text{DE}}(\varpi_0, x)}{\mu + x} dx \right]^{-1}, \quad (\varpi_0 = 1 - \delta), \quad (9)$$

to polish the values of  $H^{\text{DE}}(\varpi_0, \mu)$  to get a refined set of values  $H^{\text{It}}(\varpi_0, \mu)$ . Needless to say, both  $H^{\text{It}}(\varpi_0, \mu)$  and  $H^{\text{DE}}(\varpi_0, \mu)$  must be in agreement with each other to 15 digits or more provided that the latter actually approximates the true solution for the  $H$ -function with a 15-digit accuracy, and that the integration over  $x$  in Eq.(9) has been done with a comparable accuracy by means of the DE-formula. An estimation of the numerical error in each value of  $H^{\text{DE}}(\varpi_0, \mu)$  may then be made by calculating the difference of the two:

$$\Delta = [H^{\text{DE}}(\varpi_0, \mu) - H^{\text{It}}(\varpi_0, \mu)] \times 10^{15}. \quad (10)$$

Although not explicitly indicated here for brevity, the quantity  $\Delta$  depends not only on  $\varpi_0$  and  $\mu$  but also on

the values of  $\varepsilon$  and  $x_t$  assumed for the  $H$ -function calculations. The multiplicative factor  $10^{15}$  is to stress how many units of difference exist in the figure at the 15-th decimal place of a given value of  $H^{\text{DE}}(\varpi_0, \mu)$  compared with that of  $H^{\text{It}}(\varpi_0, \mu)$ , presumably a closer approximation for the true value.

For the purpose of an additional check, we shall also calculate the zeroth through fourth order moments  $\alpha_m(\varpi_0)$  ( $m = 0, \dots, 4$ ) of the  $H$ -function:

$$\alpha_m(\varpi_0) = \int_0^1 H^{\text{DE}}(\varpi_0, x) x^m dx, \quad (m = 0, 1, 2, 3, 4), \quad (11)$$

which yields the following analytical relations:

$$\alpha_0(\varpi_0) = \begin{cases} (2/\varpi_0)[1 - \sqrt{\delta}], & (\varpi_0 = 1 - \delta), \\ (128 + \varpi_0(32 + \varpi_0(16 + \varpi_0(10 + \\ + 7\varpi_0))))/128, & (\varpi_0 \leq 10^{-3}), \end{cases} \quad (12)$$

together with

$$\alpha_0(1) = 2, \quad (13a)$$

$$\alpha_1(1) = 2/\sqrt{3} = 1.154700538379251 \dots, \quad (13b)$$

$$\alpha_2(1) = 2q_\infty/\sqrt{3} = 0.8203524821491256 \dots, \quad (13c)$$

$$\alpha_3(1) = \left( \frac{1}{3} q_\infty^2 + \frac{1}{5} \right) \sqrt{3} = 0.6378182680315181 \dots, \quad (13d)$$

where the second expression of Eq.(12) is based on the series expansion of  $\sqrt{1 - \varpi_0}$  with respect to  $\varpi_0$  to the term of order  $\varpi_0^5$ , and the quantity  $q_\infty$  is the Hopf constant (Yanovitskij 1997) or the Hopf extrapolation length (van de Hulst 1980), whose value 0.71044608959876307... is given by Viik (1986) up to the 59-th decimal place (see also Appendix of the present work). The numerical integrations required for Eq.(11) are to be carried out also using the DE-formula to achieve as high an accuracy as possible.

### 3 Numerical Results

A foremost reference of comparison to judge the quality of our numerical results would be Table XI on p. 125 of Chandrasekhar (1960). Unfortunately, however, some of the numerical values presented in this table contain non-negligible errors in the fourth or fifth decimal figures as has already been noted by Hiroi (1994). Since his tabulation fully covers Table XI but with higher numerical accuracy, we instead made a direct comparison of our results with those of Hiroi (1994) by adopting all

of the 47  $\varpi_0$ -values employed by him for tabulation together with nine additional values, viz.,  $10^{-3}$ ,  $1 - 10^{-5}$ ,  $1 - 10^{-7}$ ,  $1 - 10^{-9}$ ,  $1 - 10^{-10}$ ,  $1 - 10^{-11}$ ,  $1 - 10^{-12}$ ,  $1 - 10^{-13}$ , and  $1 - 10^{-14}$  to inspect the behavior of our values of the  $H$ -function in the presence of strong extinction or in the near-conservative cases. For each of these, the values of the  $H$ -function were calculated at 22 values of  $\mu$  comprising 21 values 0 (0.05) 1 employed by Hiroi (1994) also for his tabulation and one extra value 0.01.

For a given set of values for the parameters  $(\varepsilon, x_t)$ ,  $56 \times 22$  absolute values of  $\Delta$  were obtained following Eq.(10), which were then summed up to get the total value  $\Delta^{\text{Tot}}(\varepsilon, x_t)$ :

$$\Delta^{\text{Tot}}(\varepsilon, x_t) = \sum_{\varpi_0, \mu} |\Delta| \quad (14)$$

It is expected that the set of values for  $(\varepsilon, x_t)$  which minimizes the value of  $\Delta^{\text{Tot}}(\varepsilon, x_t)$  is optimal. We made a search for such pair incorporating the subroutine *powell* in Press et al. (1992) with our FORTRAN code for  $H^{\text{DE}}(\varpi_0, \mu)$  calculations and treating the  $\Delta^{\text{Tot}}(\varepsilon, x_t)$  as the target function, to get to the following result:

$$\begin{aligned} \varepsilon &= 6.009587099094104 \times 10^{-3}, \\ x_t &= 1.238798627279953 \times 10^{-1}, \end{aligned} \quad (15)$$

which we adopted to generate the final version of numerical tables of  $H^{\text{DE}}(\varpi_0, \mu)$ .

To start with, our numerical results, rounded to the fifth decimal place, were compared with those of Hiroi (1994) shown at 987 ( $= 47 \times 21$ ) entries in his Table 1: the figures in the two data sets were in perfect agreement at 966 entries, and one unit differences in the fifth decimal possibly arising from round-off errors were found at the remaining 21 entries. In contrast, Table XI of Chandrasekhar (1960) exhibits numerous differences in the fifth or even in the fourth decimal compared to ours: for  $\varpi_0 = 0.7$  and  $\mu = 0.05$ , for instance, we as well as Hiroi (1994) have 1.06765, whereas Chandrasekhar (1960) gives 1.06780. In view of the fact that our result and Hiroi's are identical in spite of the difference in the adopted computational methods, this difference of 0.00015 can duly be attributed to a fourth decimal error involved in the value shown in Chandrasekhar's Table XI.

Tables 1 through 6 show the values of  $H^{\text{DE}}(\varpi_0, \mu)$  to the 15-th decimal place (16 decimal digits) as functions of  $\varpi_0$  and  $\mu$ : 18 values of  $\varpi_0$ , viz.,  $10^{-3}$ , 0.1, 0.3, 0.5, 0.7, 0.8, 0.9, 0.99, 0.999,  $1 - 10^{-5}$ ,  $1 - 10^{-7}$ ,  $1 - 10^{-9}$ ,  $1 - 10^{-10}$ ,  $1 - 10^{-11}$ ,  $1 - 10^{-12}$ ,  $1 - 10^{-13}$ ,  $1 - 10^{-14}$ , and 1, selected from the 56, and the 22 aforementioned values of  $\mu$ , viz., 0, 0.01, and 0.05 (0.05) 1 adopted for

our calculations. For brevity, however, we have dropped the suffix DE in the tabulation.

The value of  $\Delta$  associated with each value of  $H^{\text{DE}}(\varpi_0, \mu)$  indicates a possible error present in the 15-th decimal figure. We see that the largest magnitude of error is 2, so that all the results for  $H^{\text{DE}}(\varpi_0, \mu)$  must be exact at least to the 14-th decimal place or to 15 decimal digits.<sup>2</sup> Also shown in the bottom section of each table are the values calculated for the zeroth through fourth order moments  $\alpha_m(\varpi_0)$  ( $m = 0, \dots, 4$ ) of the  $H^{\text{DE}}(\varpi_0, \mu)$  as functions of  $\varpi_0$ .

As a second check, we compared our values for  $H^{\text{DE}}(\varpi_0, \mu)$  and  $\alpha_m(\varpi_0)$  ( $m = 0, \dots, 4$ ) with those tabulated in Bosma and de Rooij (1983) to the 10-th decimal place, to confirm that both data sets fully agree with each other if ours are rounded to the 10-th decimal place. Next, our results for  $\alpha_0(\varpi_0)$  and  $\alpha_m(1)$  ( $m = 1, 2, 3$ ) were compared with those given by Eqs.(12) and (13), to find that they too are in perfect agreement with each other to the 15-th decimal place.

We should also note that Viik (1986) gives in his TABLE II the values of the  $H$ -function for isotropic scattering at 11 values of  $\mu$ , viz., 0 (0.1) 1, for two values of  $\varpi_0$ , viz., 0.5 and 1, to the 13-th decimal place. The values for  $H^{\text{DE}}(\varpi_0, \mu)$  agree with his to the last figures except that ours are larger by one unit in the last decimal place at  $\mu = 0.2, 0.4, 0.6$ , and  $0.7$  in the case of  $\varpi_0 = 0.5$  due probably to round-off errors. In addition, all our results for  $\alpha_m(\varpi_0)$  ( $m = 0, 1, 2$ ) for  $\varpi_0 = 0.5$  and 1 are also found to agree with those of Viik (1986) to the 13-th decimal place; an exception is our value of  $\alpha_1(1)$ , which is larger by one unit than Viik's in the 13-th decimal place again due possibly to a round-off error.

It may be worth noting that even with the 350-point Gauss-Legendre quadrature, Kawabata and Limaye (2011) had some difficulty in getting the value of  $\alpha_0(\varpi_0)$  correct to the 10-th decimal place for some values of  $\varpi_0$  quite in contrast to the present work where we have experienced no such problem under the DE-formula.

## 4 Conclusion

We have developed a numerical scheme to calculate values of Chandrasekhar's  $H$ -function for isotropic scattering with 15-digit accuracy. The important elements of this scheme can be summarized as following:

<sup>2</sup>The magnitudes of errors are compiler-dependent. If we run the same FORTRAN code using, e.g., the GFORTRAN Ver. 4.8.1 for 32-bit computers, we get the maximum error of 4 in the 15-th decimal.

1. The closed form integral representation for the  $H$ -function is employed as in Kawabata and Limaye (2011).
2. The Gauss-Legendre quadrature adopted by Kawabata and Limaye (2011) is replaced with the double exponential formula (DE-formula) of Takahashi and Mori (1974) that enables us to perform the required integrations with considerably higher accuracy. In creating our FORTRAN code, we gratefully benefited from the automatic integrator routine *DEAUTO* written by Watanabe (1990) in RATFOR, which ingeniously circumvents the over-flow problem frequently encountered in calculating the quadrature weights. We retain all his input parameter values also in our calculations.
3. In the case of conservative scattering ( $\varpi_0 = 1$ ), an analytical integration based on the Maclaurin series expansion of the integrand is used as in Kawabata and Limaye (2011) for the integration over a small interval  $[0, \varepsilon]$  ( $\varepsilon \ll 1$ ) to reduce numerical inaccuracy that is likely to be introduced by the logarithmic divergence of the integrand, whereas the DE-formula is applied to the integration over the remaining interval  $[\varepsilon, \pi/2]$ . In the cases of non-conservative scattering ( $\varpi_0 < 1$ ), on the other hand, only the DE-formula is applied to the entire single interval  $[0, \pi/2]$ .
4. In the interval  $[0, x_t]$  ( $x_t < 1$ ), where  $x_t$  is a prescribed demarcation point, the function  $1 - \varpi_0 x / \tan x$  in the integrand is approximated by the Maclaurin series expansion terminated at the  $x^{12}$ -order term. For small values of  $x$ , this should help reduce any ill-effect that would arise from the inaccuracy involved in returned values from a library function  $\tan(x)$  supplied by a compiler in use. In addition, especially for  $\varpi_0 > 0.999$ , it is crucial to first specify the residue  $\delta = 1 - \varpi_0$ , and subsequently calculate the value of  $\varpi_0 (= 1 - \delta)$  in order to avoid loss of significant figures which inevitably occurs in calculating  $1 - \varpi_0$  whenever  $\varpi_0$  is close to unity.

In contrast, for  $\varpi_0 \leq 10^{-3}$ , the exact value of  $\alpha_0(\varpi_0)$  can better be evaluated with an approximate representation like the second one of Eq.(12), although our numerical calculations of the moments using Eq.(11) are hardly affected under such circumstances.

5. Accuracy of the calculated values for the  $H$ -function was found to depend on the chosen values for the parameters  $(\varepsilon, x_t)$ . A set of optimum values for them was therefore searched using a modified Powell method for function minimization: the quantity  $\Delta^{\text{Tot}}(\varepsilon, x_t)$  (see Eq.(14)) was thereby employed as the target function.

With the optimum values obtained for  $(\varepsilon, x_t)$ , we carried out calculations of the numerical values of the  $H$ -function for combinations of 56 values of  $\varpi_0$  and 22 values of  $\mu$ . The results for 18 selected values of  $\varpi_0$  are presented in Tables 1 through 6. The magnitudes of errors involved in our results are estimated to be at most 2 in the 15-th decimal places. In other words, our values of the  $H$ -function for isotropic scattering  $H^{\text{DE}}(\varpi_0, \mu)$  are supposed to be correct at least to the 14-th decimal place or 15 digits.

The DE-formula is also capable of yielding numerical values for the zeroth moment  $\alpha_0(\varpi_0)$  to the 15-th decimal place in comparison with the exact values. As for the first through fourth order moments  $\alpha_m(\varpi_0)$  ( $m = 1, \dots, 4$ ), our values are obviously correct at least to the 10-th decimal place as the comparison with those of Bosma and de Rooij (1983) indicates. It is highly likely that they are correct even to the 15-th decimal in view of the fact that ours for  $\alpha_1(1)$ ,  $\alpha_2(1)$ , and  $\alpha_3(1)$  agree perfectly with the exact values and that our values of  $\alpha_m(0.5)$  ( $m = 0, 1, 2$ ) coincide with those of Viik (1986) to the 13-th decimal.

**Acknowledgements** The author is grateful to the anonymous reviewer for his or her valuable suggestions.

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## A Expansion coefficients for the Hopf constant

The Hopf constant  $q_\infty$  can be calculated using the formula by Placzek and Seidel(1947):

$$q_\infty = \frac{6}{\pi^2} + \frac{1}{\pi} \int_0^{\pi/2} \left( \frac{3}{x^2} - \frac{1}{1 - x \cot x} \right) dx. \quad (\text{A1})$$

Following Viik(1986), we expand the integrand of Eq.(A1) in a power series of  $x$  up to the term of  $x^n$ , and carry out the integration analytically, to get the following result:

$$q_\infty \simeq \frac{6}{\pi^2} + \frac{1}{\pi} \sum_{n=2}^{\infty} \frac{(-b_n)}{2n-3} \left( \frac{\pi}{2} \right)^{2n-3}, \quad (\text{A2})$$

It is found that terminating the series at  $n = 250$ , the numerical value given by Viik (1986) can be reproduced to the 59-th decimal place by rounding off the

60-th decimal figure 8 of our result:

$$\begin{aligned} &0.7104460895987630727325241416991536719932 \\ &01333958785239092798 \end{aligned} \quad (\text{A3})$$

(see also Loyalka and Naz 2006, which gives this value to the 20-th decimal place).

We present in Table 7 the coefficients  $(-b_n)$  up to  $n = 17$  in fraction form, ignoring all the terms beyond  $(\pi/2)^{33}$ , and in Table 8 in decimal form. We have confirmed that the value of  $q_\infty$  can be reproduced to the 15-th decimal figure or 0.7104460895987631 using a FORTRAN code in double-precision arithmetic by incorporating the coefficients given in Table 8. It must also be noted that the values for  $b_n$  ( $n = 2, 3, 4, 5$ ) shown here are in full agreement with those cited in Viik(1986).

**Table 1**  $H(\varpi_0, \mu)$  for isotropic scattering obtained by DE-formula

$\mu$	$\varpi_0 = 0.001$	$\Delta$	$\varpi_0 = 0.1$	$\Delta$	$\varpi_0 = 0.3$	$\Delta$
0.00	1.000000000000000	0	1.000000000000000	0	1.000000000000000	0
0.01	1.000023079276825	0	1.002345867956824	0	1.007302106320789	0
0.05	1.000076131960432	0	1.007808971225585	0	1.024805080799005	0
0.10	1.000119931789617	0	1.012378097521557	0	1.039874888488393	0
0.15	1.000152819807939	0	1.015841506268183	0	1.051546361588496	0
0.20	1.000179244792271	0	1.018644075804065	-1	1.061146531525849	0
0.25	1.000201262444438	0	1.020992537960899	0	1.069298694975040	0
0.30	1.000220045948286	0	1.023005563463196	0	1.076364959992271	0
0.35	1.000236344202557	0	1.024759334758916	0	1.082580630562847	0
0.40	1.000250670335105	0	1.026306329929175	0	1.088109725497495	1
0.45	1.000263393666112	0	1.027684508780403	0	1.093072235673804	1
0.50	1.000274789867379	0	1.028922337487161	0	1.097559108679834	0
0.55	1.000285070583005	0	1.030041764949414	0	1.101641177067604	0
0.60	1.000294401997181	0	1.031060094515257	0	1.105374809040979	0
0.65	1.000302917028510	0	1.031991217231523	0	1.108805656809118	0
0.70	1.000310723643944	0	1.032846455396843	0	1.111971238341045	0
0.75	1.000317910704164	0	1.033635157555853	0	1.114902771206713	0
0.80	1.000324552180561	0	1.034365129091853	0	1.117626509039725	0
0.85	1.000330710264780	0	1.035042950713589	-1	1.120164736919162	0
0.90	1.000336437705311	0	1.035674218484590	0	1.122536526665526	0
0.95	1.000341779592330	0	1.036263727699855	0	1.124758319300910	0
1.00	1.000346774740928	0	1.036815615781196	0	1.126844380631286	0
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$\alpha_0$	1.000250125078180		1.026334038989724		1.088933156439496	
$\alpha_1$	0.500147794234295		0.515610619015497		0.553121064485779	
$\alpha_2$	0.333437556858291		0.344358308240080		0.370984157353370	
$\alpha_3$	0.250080340576093		0.258505711234432		0.279106127488061	
$\alpha_4$	0.200065314263529		0.206918528053885		0.223705287319367	



**Table 2**  $H(\varpi_0, \mu)$  for isotropic scattering obtained by DE-formula

$\mu$	$\varpi_0 = 0.5$	$\Delta$	$\varpi_0 = 0.7$	$\Delta$	$\varpi_0 = 0.8$	$\Delta$
0.00	1.000000000000000	0	1.000000000000000	0	1.000000000000000	0
0.01	1.012723830480086	0	1.018874827015222	0	1.022420537254950	0
0.05	1.044265160581558	0	1.067654600041384	0	1.081914516266725	1
0.10	1.072368762029909	0	1.113031838677712	-1	1.138807666285126	0
0.15	1.094709732081995	0	1.150343829254924	0	1.186640082601294	0
0.20	1.113461428850377	0	1.182515785241134	0	1.228638765535220	0
0.25	1.129653093499740	0	1.210934115182344	0	1.266322487667053	0
0.30	1.143889508574922	0	1.236419324639275	0	1.300588278431887	0
0.35	1.156568713007439	0	1.259517410773021	0	1.332034056023601	0
0.40	1.167971849776487	0	1.280619201798580	0	1.361089701705004	0
0.45	1.178307321633036	0	1.300018686516232	0	1.388080645843600	0
0.50	1.187735132670431	1	1.317945063118267	0	1.413262569404318	0
0.55	1.196381452566946	0	1.334581891862322	0	1.436842021994347	0
0.60	1.204347883597196	1	1.350079291216666	0	1.458989490017426	0
0.65	1.211717646238803	0	1.364562099754409	0	1.479848112148857	1
0.70	1.218559869097970	0	1.378135560424163	0	1.499539735979634	0
0.75	1.224932658619432	0	1.390889410611728	0	1.518169271958706	0
0.80	1.230885353499438	0	1.402900906035831	0	1.535827913161673	0
0.85	1.236460217044641	0	1.414237108074479	0	1.552595573997779	0
0.90	1.241693731628014	0	1.424956647948121	0	1.568542775461757	0
0.95	1.246617604949040	0	1.435111110389834	0	1.583732128410658	0
1.00	1.251259563383223	1	1.444746134765130	0	1.598219518533160	1
$\alpha_0$	1.171572875253810		1.292221264270954		1.381966011250105	
$\alpha_1$	0.603484255848994		0.678667819110035		0.735815233031298	
$\alpha_2$	0.407023642126835		0.461419889227813		0.503223793206828	
$\alpha_3$	0.307119523431517		0.349675124789374		0.382595118839524	
$\alpha_4$	0.246600776618178		0.281528145681548		0.308664834854489	

**Table 3**  $H(\varpi_0, \mu)$  for isotropic scattering obtained by DE-formula

$\mu$	$\varpi_0 = 0.9$	$\Delta$	$\varpi_0 = 0.99$	$\Delta$	$\varpi_0 = 0.999$	$\Delta$
0.00	1.000000000000000	0	1.000000000000000	0	1.000000000000000	0
0.01	1.026603764674318	0	1.032257470361386	0	1.033674233753012	0
0.05	1.099678288027236	1	1.126070564855184	0	1.133393124789600	0
0.10	1.172143053516453	0	1.224875290417156	0	1.240424772856097	-1
0.15	1.234918332479768	0	1.314972472230572	0	1.339648497723789	0
0.20	1.291433728065182	0	1.399767224074789	0	1.434415855969377	0
0.25	1.343270825469927	0	1.480742606314496	1	1.526164843765312	0
0.30	1.391350320632572	0	1.558712877184762	0	1.615671055040806	1
0.35	1.436280343349813	0	1.634185389649200	1	1.703407663333851	0
0.40	1.478496236155405	0	1.707503465981193	0	1.789687085591210	0
0.45	1.518327492340675	1	1.778913614217836	1	1.874727429567537	1
0.50	1.556033802021363	0	1.848601016447846	1	1.958687474359325	0
0.55	1.591826182604205	0	1.916709878377813	0	2.041686670750376	0
0.60	1.625880196208851	0	1.983355849810225	0	2.123817312270080	0
0.65	1.658344654834039	0	2.048633986828251	0	2.205152313093988	0
0.70	1.689347600330646	1	2.112624062808928	1	2.285750378701103	0
0.75	1.719000559169012	0	2.175394229576233	1	2.365659557180583	-1
0.80	1.747401661141401	0	2.237003612379969	0	2.444919746120597	0
0.85	1.774637984393825	1	2.297504193613621	0	2.523564504125438	0
0.90	1.800787358056601	0	2.356942208926965	0	2.601622386587422	0
0.95	1.825919774834691	0	2.415359201062581	1	2.679117948214393	0
1.00	1.850098516769812	-1	2.472792828397026	0	2.756072507268736	0
$\alpha_0$	1.519493853295915		1.818181818181818		1.938693139936569	
$\alpha_1$	0.825315748434260		1.027181735489862		1.111330550198365	
$\alpha_2$	0.569448617885390		0.721955096966521		0.786717738091024	
$\alpha_3$	0.435113601428221		0.557657562330954		0.610325627802045	
$\alpha_4$	0.352161961828424		0.454579895752381		0.498970970855085	

**Table 4**  $H(\varpi_0, \mu)$  for isotropic scattering obtained by DE-formula

$\mu$	$\varpi_0 = 1 - 10^{-5}$	$\Delta$	$\varpi_0 = 1 - 10^{-7}$	$\Delta$	$\varpi_0 = 1 - 10^{-9}$	$\Delta$
0.00	1.000000000000000	0	1.000000000000000	0	1.000000000000000	0
0.01	1.034205719689598	0	1.034256922275328	0	1.034262022863829	1
0.05	1.136262879388996	0	1.136543713405656	0	1.136571734129853	0
0.10	1.246666275155322	0	1.247282112614023	0	1.247343610377832	0
0.15	1.349722855408363	0	1.350722601325096	0	1.350822494497537	0
0.20	1.448762094088692	0	1.450192529327167	0	1.450335524951871	0
0.25	1.545207661341358	0	1.547114359446071	0	1.547305046360939	0
0.30	1.639824632440255	0	1.642252383517436	0	1.642495275204116	0
0.35	1.733077835787557	0	1.736070880193769	0	1.736370438341392	1
0.40	1.825272706424626	0	1.828874877403022	-1	1.829235526266891	0
0.45	1.916621283338394	0	1.920876100191321	0	1.921302235960664	1
0.50	2.007276919589851	0	2.012227651599931	1	2.012723648818164	1
0.55	2.097354110520160	0	2.103043822474229	0	2.103614038607345	1
0.60	2.186940550203905	0	2.193412135789794	0	2.194060914574986	0
0.65	2.276104830260681	0	2.283401037166935	1	2.284132711127234	0
0.70	2.364901554295879	1	2.373065003460309	1	2.373883895831389	1
0.75	2.453374848241580	-1	2.462448048868194	1	2.463358475100236	0
0.80	2.541560836748558	0	2.551586198198066	0	2.552592467143796	1
0.85	2.629489431573132	-1	2.640509272900804	0	2.641615687767435	0
0.90	2.717185649514410	0	2.729242207208971	1	2.730453066329686	0
0.95	2.804670600985655	1	2.817806035313179	2	2.819125632778694	0
1.00	2.891962243185030	-2	2.906218643437432	0	2.907651269617728	-1
$\alpha_0$	1.993695381633480		1.999367744404741		1.999936756446733	
$\alpha_1$	1.150223392945239		1.154251374421934		1.154655607439818	
$\alpha_2$	0.816872433717816		0.820003269398072		0.820317548751288	
$\alpha_3$	0.634969398790733		0.637532347623988		0.637789665617137	
$\alpha_4$	0.519814783449839		0.521985149313924		0.522203079284880	

**Table 5**  $H(\varpi_0, \mu)$  for isotropic scattering obtained by DE-formula

$\mu$	$\varpi_0 = 1 - 10^{-10}$	$\Delta$	$\varpi_0 = 1 - 10^{-11}$	$\Delta$	$\varpi_0 = 1 - 10^{-12}$	$\Delta$
0.00	1.000000000000000	0	1.000000000000000	0	1.000000000000000	0
0.01	1.034262410233136	0	1.034262532725766	0	1.034262571460906	0
0.05	1.136573862529025	1	1.136574535574220	0	1.136574748408426	0
0.10	1.247348282010408	-1	1.247349759291493	0	1.247350226446905	0
0.15	1.350830083242122	0	1.350832482995976	0	1.350833241862986	0
0.20	1.450346388639971	1	1.450349824029179	0	1.450350910393573	0
0.25	1.547319533862394	0	1.547324115216175	0	1.547325563967803	0
0.30	1.642513729686032	0	1.642519565530900	0	1.642521410989613	0
0.35	1.736393199059862	1	1.736400396686262	0	1.736402672781104	1
0.40	1.829262929658623	-1	1.829271595466160	0	1.829274335844537	0
0.45	1.921334616355098	0	1.921344856077736	0	1.921348094176634	0
0.50	2.012761338925487	0	2.012773257785881	1	2.012777026880672	1
0.55	2.103657369865718	1	2.103671072685019	0	2.103675405924182	0
0.60	2.194110217405046	0	2.194125808683393	0	2.194130739113968	-1
0.65	2.284188315123211	0	2.284205899100158	1	2.284211459686857	0
0.70	2.373946129907529	0	2.373965810608357	0	2.373972034248210	0
0.75	2.463427667604941	0	2.463449548876749	1	2.463456468410514	0
0.80	2.552668945949899	0	2.552693131490155	-1	2.552700779711349	0
0.85	2.641699780344541	0	2.641726373723957	1	2.641734783386086	0
0.90	2.730545099802790	0	2.730574204483862	1	2.730583408306289	0
0.95	2.819225933976175	0	2.819257653328354	0	2.819267684001096	1
1.00	2.907760165110989	0	2.907794602423222	-1	2.907805492610912	0
$\alpha_0$	1.999980000199998		1.999993675464680		1.999998000002000	
$\alpha_1$	1.154686329619116		1.154696045139821		1.154699117488689	
$\alpha_2$	0.820341434947413		0.820348988688071		0.820351377416827	
$\alpha_3$	0.637809222904595		0.637815407686305		0.637817363508448	
$\alpha_4$	0.522219643112460		0.522224881250612		0.522226537714934	

**Table 6**  $H(\varpi_0, \mu)$  for isotropic scattering obtained by DE-formula

$\mu$	$\varpi_0 = 1 - 10^{-13}$	$\Delta$	$\varpi_0 = 1 - 10^{-14}$	$\Delta$	$\varpi_0 = 1$	$\Delta$
0.00	1.000000000000000	0	1.000000000000000	0	1.000000000000000	0
0.01	1.034262583709990	0	1.034262587583486	0	1.034262589374882	0
0.05	1.136574815712375	0	1.136574836995738	0	1.136574846838766	0
0.10	1.247350374174229	0	1.247350420889692	0	1.247350442494436	0
0.15	1.350833481837627	0	1.350833557724253	0	1.350833592819941	1
0.20	1.450351253932052	0	1.450351362568447	-1	1.450351412810095	0
0.25	1.547326022103329	0	1.547326166978507	0	1.547326233979698	0
0.30	1.642521994575152	0	1.642522179121128	0	1.642522264469087	-1
0.35	1.736403392546043	0	1.736403620155757	0	1.736403725419636	0
0.40	1.829275202429211	-1	1.829275476467441	0	1.829275603203367	-1
0.45	1.921349118154844	0	1.921349441965328	0	1.921349591719701	0
0.50	2.012778218775117	0	2.012778595685436	0	2.012778769997181	0
0.55	2.103676776217445	-1	2.103677209542494	-1	2.103677409944670	0
0.60	2.194132298256560	0	2.194132791301094	1	2.194133019322067	0
0.65	2.284213218103263	0	2.284213774163804	0	2.284214031328140	0
0.70	2.373974002341517	-1	2.373974624707825	0	2.373974912536958	0
0.75	2.463458656566025	0	2.463459348522235	1	2.463459668534998	0
0.80	2.552703198299433	0	2.552703963124959	0	2.552704316838003	1
0.85	2.641737442764470	0	2.641738283734728	1	2.641738672662854	0
0.90	2.730586318821909	0	2.730587239208903	-1	2.730587664865336	0
0.95	2.819270855991615	1	2.819271859064420	1	2.819272322961027	0
1.00	2.907808936405973	-1	2.907810025431127	0	2.907810529078606	0
$\alpha_0$	1.999999367544668		1.999999800000020		2.000000000000000	
$\alpha_1$	1.154700089053853		1.154700396290050		1.154700538379251	
$\alpha_2$	0.820352132801808		0.820352371675775		0.820352482149125	
$\alpha_3$	0.637817981995959		0.637818177579107		0.637818268031518	
$\alpha_4$	0.522227061536906		0.522227227184154		0.522227303791946	

**Table 7** Expansion coefficients for the Hopf constant  $q_\infty$  in fraction form

$n$	$2n - 3$	$-b_n$
2	1	$1/5$
3	3	$1/175$
4	5	$2/7875$
5	7	$37/3031875$
6	9	$118/197071875$
7	11	$5506/186232921875$
8	13	$3308/2261399765625$
9	15	$8386459/115794974998828125$
10	17	$56067454/15632321624841796875$
11	19	$29059045766/163592245803969404296875$
12	21	$654185668/74360111729077001953125$
13	23	$94994770034/218018127581059225341796875$
14	25	$682205256508/31612628499253587674560546875$
15	27	$8101862427463268/7580234124693521520544500732421875$
16	29	$2112667618521098312/39909932666511390805666796356201171875$
17	31	$765408870503963716543/291941157455530823743452615345611572265625$

**Table 8** Expansion coefficients for the Hopf constant  $q_\infty$  in decimal form

$n$	$-b_n$	$n$	$-b_n$
1	3	11	1.776309483569356(−13)
2	2.000000000000000(−1) <sup>a</sup>	12	8.797534764114590(−15)
3	5.714285714285714(−3)	13	4.357195939988105(−16)
4	2.539682539682540(−4)	14	2.158014973427811(−17)
5	1.220366934652649(−5)	15	1.068814273304630(−18)
6	5.987663130520273(−7)	16	5.293588531392957(−20)
7	2.956512707079601(−8)	17	2.621791586958932(−21)
8	1.462810799878960(−9)		
9	7.242506853242011(−11)		
10	3.586636415598148(−12)		

<sup>a</sup>This is to read as  $2.000000000000000 \times 10^{-1}$ .